PFHxS

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2150 L/kg

Global applicability domain: Outside

Local applicability domain index: 2.96e-01

Confidence level: 6.61e-01

Nearest Neighbors from the Training Set

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Tetrachlorovinphos	Z-Tetrachlorvinphos	Chlorthal-dimethyl
Measured: 1020	**Measured:** 1020	**Measured:** 5010
Predicted: 1070	**Predicted:** 1070	**Predicted:** 2160

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Tetrachlorophthalic acid	Fthalide	Niclosamide
Measured: 2000	**Measured:** 2000	**Measured:** 2240
Predicted: 1980	**Predicted:** 1600	**Predicted:** 4670